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chain bonds :
4-7  6-8  8-9  9-10  10-11
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6
exact/norm bonds :
1-2  1-6  2-3  3-4  4-5  4-7  5-6  10-11
exact bonds :
6-8  8-9  9-10

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:CLASS  8:CLASS  9:CLASS  10:CLASS
 11:CLASS



L1      STRUCTURE UPLOADED

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L1              STR
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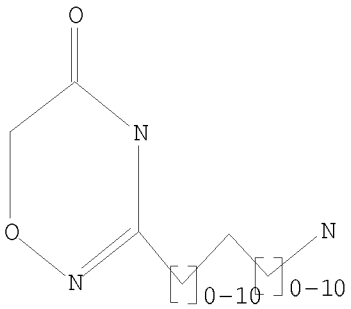


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Structure attributes must be viewed using STN Express query preparation.


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SAMPLE SCREEN SEARCH COMPLETED -        8 TO ITERATE

100.0% PROCESSED        8 ITERATIONS                                0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:             8 TO      329
PROJECTED ANSWERS:                0 TO        0

L2            0 SEA SSS SAM L1

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FULL SEARCH INITIATED 09:13:56 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -      205 TO ITERATE
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100.0% PROCESSED 205 ITERATIONS 21 ANSWERS
SEARCH TIME: 00.00.01

L3 21 SEA SSS FUL L1

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COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 185.88 186.10

FILE 'CAPLUS' ENTERED AT 09:14:00 ON 12 JAN 2009
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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FILE COVERS 1907 - 12 Jan 2009 VOL 150 ISS 3
FILE LAST UPDATED: 11 Jan 2009 (20090111/ED)

Caplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

http://www.cas.org/legal/infopolicy.html

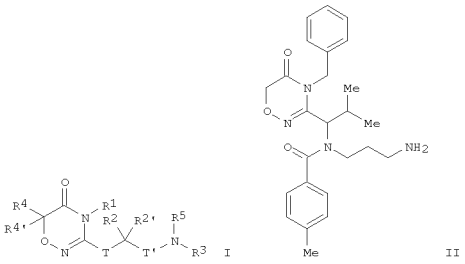
=> s l3
L4 3 L3

=> d ibib abs hitstr tot

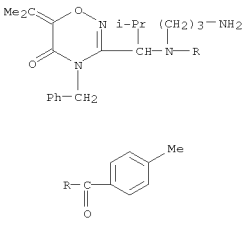
L4 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2004:902133 CAPLUS
DOCUMENT NUMBER: 141:379946
TITLE: Preparation of 5,6-dihydro-4H-1,2,4-oxadiazin-5-ones as KSP inhibitors for treatment of cellular proliferative diseases
INVENTOR(S): Qian, Xiangping; Bergnes, Gustave; Morgans, David J.
PATENT ASSIGNEE(S): Cytokinetics, Inc, USA
SOURCE: PCT Int. Appl., 97 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004091547	A2	20041028	WO 2004-US9274	20040409
WO 2004091547	A3	20050506		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1622883	A2	20060208	EP 2004-758979	20040409
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
JP 2006523232	T	20061012	JP 2006-509333	20040409
US 20070232597	A1	20071004	US 2006-552611	20060920
PRIORITY APPLN. INFO.:			US 2003-462077P P	20030410
			WO 2004-US9274 W	20040409

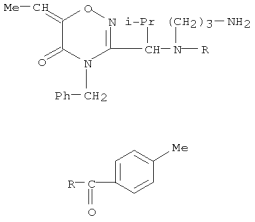
OTHER SOURCE(S): MARPAT 141:379946
GI



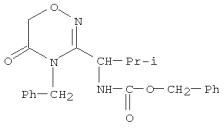
AB Title compds. I [wherein T, T' = independently a bond, (un)substituted alkylene; R1, R2, R2', R4, R4', R5, R8 = independently H, (un)substituted alkyl, (hetero)aryl(alkyl); R3 = H, (un)substituted alkyl, (hetero)aryl(alkyl), COR6, SO2R6a; or CR2R2', NR3R5, or NT'CR2R5 = (un)substituted heterocyclyl; or CR4R4' = (un)substituted cycloalkyl; R6 = H, (un)substituted alkyl, (hetero)aryl(alkyl), OR7, NHR8; R6a = (un)substituted alkyl, (hetero)aryl(alkyl), NHR8; R7 = (un)substituted alkyl, (hetero)aryl(alkyl); and pharmaceutically acceptable salts or solvates thereof] were prepared as KSP inhibitors. For example, a 7-step synthesis starting from CBZ-valine, benzylamine, (aminooxy)acetic acid, 3-(tert-butoxycarbonylamino)propanal, and p-toluoyl chloride produced II. Compds. of the invention inhibited cell proliferation with GI50 values ranging from 200 nM to >20 μM. Thus, I and their pharmaceutical compns., optionally comprising another chemotherapeutic agent, are useful for the treatment of proliferative diseases and disorders, such as cancer, hyperplasias, restenosis, cardiac hypertrophy, immune disorders, and inflammation (no data).
IT 782500-02-1P, N-(3-Aminopropyl)-N-[1-(4-benzyl-6-isopropylidene-5-oxo-5,6-dihydro-4H-[1,2,4]oxadiazin-3-yl)-2-methylpropyl]-4-methylbenzamide 782500-03-2P, N-(3-Aminopropyl)-N-[1-(4-benzyl-6-ethylidene-5-oxo-5,6-dihydro-4H-[1,2,4]oxadiazin-3-yl)-2-methylpropyl]-4-methylbenzamide
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(KSP inhibitor; preparation of oxadiazinones as KSP inhibitors for treatment of cellular proliferative diseases)
RN 782500-02-1 CAPLUS
CN Benzamide, N-(3-aminopropyl)-N-[1-[5,6-dihydro-6-(1-methylethylidene)-5-oxo-4-(phenylmethyl)-4H-1,2,4-oxadiazin-3-yl]-2-methylpropyl]-4-methyl- (CA INDEX NAME)



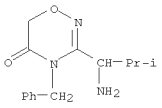
RN 782500-03-2 CAPLUS
CN Benzamide, N-(3-aminopropyl)-N-[1-[6-ethylidene-5,6-dihydro-5-oxo-4-(phenylmethyl)-4H-1,2,4-oxadiazin-3-yl]-2-methylpropyl]-4-methyl- (CA INDEX NAME)



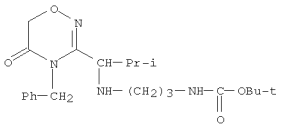
IT 782500-05-4P 782500-06-5P 782500-07-6P
782500-10-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of oxadiazinones as KSP inhibitors for treatment of cellular proliferative diseases)
RN 782500-05-4 CAPLUS
CN Carbamic acid, [1-[5,6-dihydro-5-oxo-4-(phenylmethyl)-4H-1,2,4-oxadiazin-3-yl]-2-methylpropyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)



RN 782500-06-5 CAPLUS
CN 4H-1,2,4-Oxadiazin-5(6H)-one, 3-(1-amino-2-methylpropyl)-4-(phenylmethyl)- (CA INDEX NAME)

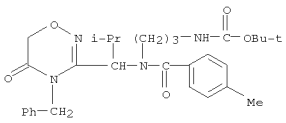


RN 782500-07-6 CAPLUS
CN Carbamic acid, [3-[[1-[5,6-dihydro-5-oxo-4-(phenylmethyl)-4H-1,2,4-oxadiazin-3-yl]-2-methylpropyl]amino]propyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 782500-10-1 CAPLUS
CN Carbamic acid, [3-[[1-[5,6-dihydro-5-oxo-4-(phenylmethyl)-4H-1,2,4-oxadiazin-3-yl]-2-methylpropyl](4-methylbenzoyl)amino]propyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)



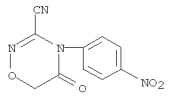
L4 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1999:710017 CAPLUS
DOCUMENT NUMBER: 132:93227
TITLE: A facile synthesis of N-arylcyanoformamidoximes, 4-aryl-3-cyano-1,2,4-oxadiazin-5(6H)-ones, 2-cyanoquinazoline-3-oxides, and 2-cyanoquinazolines via 5-arylimino-4-chloro-5H-1,2,3-dithiazoles
AUTHOR(S): Chang, Yong-Goo; Kim, Kyongtae
CORPORATE SOURCE: Department of Chemistry, Seoul National University, Seoul, 151-742, S. Korea
SOURCE: Heterocycles (1999), 51(11), 2653-2666
CODEN: HTCYAM; ISSN: 0385-5414
PUBLISHER: Japan Institute of Heterocyclic Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 132:93227

AB The reaction of 5-arylimino-4-chloro-5H-1,2,3-dithiazoles with hydroxylamine hydrochloride in pyridine at room temperature gave N-arylcyanoformamidoximes, which were utilized as starting materials for the synthesis of 4-alkyl- (or aryl)-2-cyanoquinazolines and 4-aryl-3-cyano-1,2,4-oxadiazin-5(6H)-ones.

IT 253587-37-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of arylcyanoformamidoximes, arylcyanooxadiazinones, cyanoquinazoline oxides, and cyanoquinazolines from (arylimino)chlorodithiazoles)

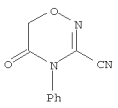
RN 253587-37-0 CAPLUS
CN 4H-1,2,4-Oxadiazine-3-carbonitrile, 5,6-dihydro-4-(4-nitrophenyl)-5-oxo- (CA INDEX NAME)



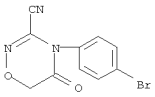
IT 253587-33-6P 253587-34-7P 253587-35-8P
253587-36-9P 253587-38-1P 253587-39-2P
253587-40-5P 253587-41-6P 253587-42-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of arylcyanoformamidoximes, arylcyanooxadiazinones, cyanoquinazoline oxides, and cyanoquinazolines from (arylimino)chlorodithiazoles)

RN 253587-33-6 CAPLUS
CN 4H-1,2,4-Oxadiazine-3-carbonitrile, 5,6-dihydro-5-oxo-4-phenyl- (CA INDEX NAME)

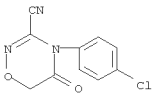
L4 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)



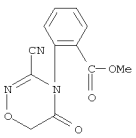
RN 253587-34-7 CAPLUS
CN 4H-1,2,4-Oxadiazine-3-carbonitrile, 4-(4-bromophenyl)-5,6-dihydro-5-oxo- (CA INDEX NAME)



RN 253587-35-8 CAPLUS
CN 4H-1,2,4-Oxadiazine-3-carbonitrile, 4-(4-chlorophenyl)-5,6-dihydro-5-oxo- (CA INDEX NAME)

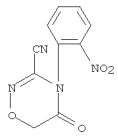


RN 253587-36-9 CAPLUS
CN Benzoic acid, 2-(3-cyano-5,6-dihydro-5-oxo-4H-1,2,4-oxadiazin-4-yl)-, methyl ester (CA INDEX NAME)

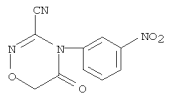


RN 253587-38-1 CAPLUS
CN 4H-1,2,4-Oxadiazine-3-carbonitrile, 5,6-dihydro-4-(2-nitrophenyl)-5-oxo- (CA INDEX NAME)

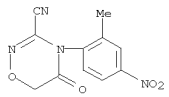
L4 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)



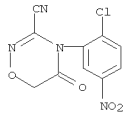
RN 253587-39-2 CAPLUS
CN 4H-1,2,4-Oxadiazine-3-carbonitrile, 5,6-dihydro-4-(3-nitrophenyl)-5-oxo- (CA INDEX NAME)



RN 253587-40-5 CAPLUS
CN 4H-1,2,4-Oxadiazine-3-carbonitrile, 5,6-dihydro-4-(2-methyl-4-nitrophenyl)-5-oxo- (CA INDEX NAME)

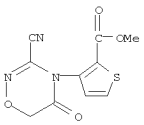


RN 253587-41-6 CAPLUS
CN 4H-1,2,4-Oxadiazine-3-carbonitrile, 4-(2-chloro-5-nitrophenyl)-5,6-dihydro-5-oxo- (CA INDEX NAME)



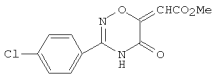
RN 253587-42-7 CAPLUS
CN 2-Thiophenecarboxylic acid, 3-(3-cyano-5,6-dihydro-5-oxo-4H-1,2,4-

L4 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)
oxadiazin-4-yl)-, methyl ester (CA INDEX NAME)



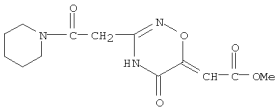
REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1979:420462 CAPLUS
DOCUMENT NUMBER: 91:20462
ORIGINAL REFERENCE NO.: 91:3425a,3428a
TITLE: Synthesis of 1,2,4-oxadiazines and their rearrangement
to pyrimidines
AUTHOR(S): Santilli, Arthur A.; Scotese, Anthony C.
CORPORATE SOURCE: Res. Dev. Div., Wyeth Lab., Inc., Radnor, PA, 19087, USA
SOURCE: Journal of Heterocyclic Chemistry (1979), 16(2), 213-16
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 91:20462
GI

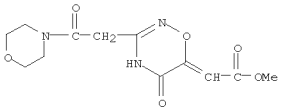


I

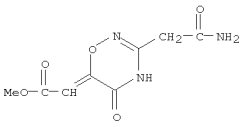
AB Several amide oximes underwent condensation reactions with MeO2CC.tplbond.CO2Me to give 1:1 adducts. Under basic conditions, these adducts underwent ring closure to give several Me [3-(substituted)-4,5-dihydro-5-oxo-6H-1,2,4-oxadiazin-6-ylidene]acetates, e.g. I. The reactions of these compds. with a variety of amines resulted in addition-rearrangement reactions with the formation of the corresponding
Me 2-substituted-5-substituted amino-1,6-dihydro-6-oxo-4-pyrimidinecarboxylates.
IT 70274-18-9P 70274-19-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and rearrangement of, pyrimidine derivative from)
RN 70274-18-9 CAPLUS
CN Acetic acid, 2-[2,5-dihydro-5-oxo-3-[2-oxo-2-(1-piperidinyl)ethyl]-6H-1,2,4-oxadiazin-6-ylidene]-, methyl ester (CA INDEX NAME)



L4 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)
RN 70274-19-0 CAPLUS
CN Acetic acid, 2-[2,5-dihydro-3-[2-(4-morpholinyl)-2-oxoethyl]-5-oxo-6H-1,2,4-oxadiazin-6-ylidene]-, methyl ester (CA INDEX NAME)



IT 70274-20-3P 70274-21-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 70274-20-3 CAPLUS
CN Acetic acid, 2-[3-(2-amino-2-oxoethyl)-2,5-dihydro-5-oxo-6H-1,2,4-oxadiazin-6-ylidene]-, methyl ester (CA INDEX NAME)



RN 70274-21-4 CAPLUS
CN Acetic acid, 2-[2,5-dihydro-3-[2-(hydroxyamino)-2-iminoethyl]-5-oxo-6H-1,2,4-oxadiazin-6-ylidene]-, methyl ester (CA INDEX NAME)